

## Electron capture into highly excited states in proton-hydrogen collisions

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(Received 10 November 1982)

A new straightforward technique for the evaluation of the rearrangement-scattering amplitude for the process  $H^+ + H(1s) \rightarrow H(nlm) + H^+$  has been presented in the continuum-intermediate-state approximation. We reduce the scattering amplitude to a closed analytical form. The asymptotic behavior of the capture cross sections with respect to  $n$  has also been derived. It has been shown conclusively that the charge-exchange cross sections asymptotically obey the  $n^{-3}$  power law throughout the entire energy range of the projectile. It is found that the cross sections for capture into different angular momentum states can be calculated from the respective asymptotic cross-section values with the help of a simple scaling law. The present calculated results have been compared with the available experimental findings.

### I. INTRODUCTION

The study of highly excited atoms formed by charge-transfer processes in ion-atom collisions has received appreciable attention both theoretically as well as experimentally in connection with their practical applications in plasma diagnostics as well as in problems connected with astrophysics. The availability of Rydberg atoms in Stellar atmospheres and interstellar space has inspired the experimental workers to produce Rydberg atoms and to study its various properties in the laboratory. The electron capture in ion-atom collisions is one of the few techniques<sup>1</sup> used for the production of Rydberg atoms in the laboratory. These highly excited atoms possess certain unusual properties due to their large size and small ionization potential. Such highly excited atoms have a fairly long lifetime against spontaneous emission and therefore are of significant importance. The cross sections for electron capture in highly excited states ( $8 \leq n \leq 25$ ) are found to have practical importance from the standpoint of laboratory production of hot plasmas.<sup>2</sup> Plasmas, in general, are produced in the laboratory from highly excited atoms in a magnetic field by injecting a fast beam of deuterium atoms. The atoms in the low-lying excited states are not fully ionized whereas the atoms in highly excited states ( $8 \leq n \leq 25$ ) are easily ionized and are suitable for the production of hot plasmas.

Recently, with the advent of sophisticated modern devices, measurement of cross sections for electron capture by protons from atomic hydrogen and molecular nitrogen in the arbitrary excited states is underway.<sup>3</sup> The calculation for electron capture into highly excited states presents formidable difficulties to a quantum mechanical treatment. This is due to the presence of a large number of oscillations in the final bound state wave function. As a result, a variety of classical and semiclassical methods<sup>2,4</sup> has been suggested by the earlier authors to study the transition between highly excited states. Recently, a few quantal calculations based on the first Born approximation (FBA),<sup>5-9</sup> the second Born approximation (SBA),<sup>10</sup> the unitarized distorted-wave approximation (UDWA),<sup>11</sup> and the eikonal approximation<sup>12</sup> (EA) are available for electron capture into highly excited states in proton-hydrogen collisions.

Although the FBA method predicts reasonable results for charge transfer in  $H^+ - H$  collisions, it is well established<sup>13-15</sup> that second-order calculations are essential in order to have a correct high-energy behavior of the charge transfer cross sections. Among the various types of second-order calculations available in the literature, cross sections for electron capture by protons from atomic hydrogen into a few low-lying excited states have been reported by the use of the impulse approximation (IA),<sup>16</sup> the eikonal approximation (EA),<sup>12,17</sup> the continuum-distorted-wave approximation (CDWA),<sup>18,19</sup> and the continuum-intermediate-state approximation (CISA).<sup>20</sup> In view of the great importance<sup>21</sup> for charge-exchange probability at large impact parameters, the EA (Ref. 22) and the CISA (Ref. 20) methods are found to be quite successful for the prediction of cross sections. The CISA method, recently developed by Belkić,<sup>20</sup> is essentially a two-state, second-order distorted-wave approximation in the impact parameter formulation. The distortion effects caused by the inclusion of continuum intermediate state are incorporated in one of the channels. The capture probability at large impact parameters obtained by the use of the CISA is in agreement with that predicted by the second Born approximation. The quantal version of the CISA has been shown<sup>23</sup> to be the rigorous first-order term of a perturbation series. The CISA method has been shown<sup>20</sup> to be more reliable than the CDWA method for describing capture at large impact parameters. Belkić<sup>20</sup> has reported cross sections for electron capture by fast protons from the ground state of atomic hydrogen into the final  $n \leq 3$  level using the CISA in the impact-energy range 25 keV–10 MeV. However, the repeated parametric differentiation technique has been used by the author to generate the relevant scattering amplitude for the calculation of cross sections. The CISA method has been found<sup>20</sup> to be in excellent agreement with measurements in the intermediate and high-energy region.

The customary procedure for the calculation of cross sections in the higher excited states by this parametric differentiation technique is not suitable from a practical point of view. This is because of the fact that the number of such differentiations increases with the increase of the principal and orbital quantum numbers. The need therefore arises for an alternative procedure which is devoid of

such difficulties and is applicable for any values of  $n$ ,  $l$ , and  $m$  including that for  $n \rightarrow \infty$ .

The present paper is aimed at developing a method for the calculation of cross sections for electron capture in arbitrary  $n$ ,  $l$ , and  $m$  states of fast protons in collision with ground-state hydrogen atoms in the framework of the CISA. The scattering amplitude has been reduced to a closed analytical form which enables one to make a comparative study of the charge transfer cross sections on the quantum numbers  $n$ ,  $l$ , and  $m$ . The behavior of the asymptotic cross section for capture into higher angular momentum states has also been investigated. Our present calculated results have been compared with the available experimental findings and other existing theoretical calculations.

The present paper is organized as follows. In Sec. II, we give the general expression for the CISA scattering amplitude for electron capture into arbitrary  $n$ ,  $l$ , and  $m$  states and then show the reduction of the scattering amplitude to a closed analytical form. The asymptotic form of the scattering amplitude has been derived in Sec. III. In Sec. IV the numerical results for the cross sections are presented and discussed. Finally, conclusions are given in Sec. V. Atomic units are used throughout the paper, unless otherwise stated.

## II. THEORY

### A. General expression for the scattering amplitude

The prior form of the CISA transition probability<sup>20,23</sup> for electron capture by fast protons from hydrogen atoms can be written as

$$T_{if} = N(v)I \cdot I', \quad (1)$$

where

$$\begin{aligned} I &= \int d\vec{x} e^{i\vec{p}\cdot\vec{x}} \Phi_i(\vec{x}) {}_1F_1(i\nu, 1; i\nu\vec{x} + i\vec{v}\cdot\vec{x}), \\ I' &= \int d\vec{s} \frac{e^{i\vec{q}\cdot\vec{s}}}{s} \Phi_f^*(\vec{s}), \\ \vec{p} &= -\vec{\eta} - \beta_1 \hat{v}, \\ \vec{q} &= \vec{\eta} + \beta_2 \hat{v}, \\ \beta_1 &= \epsilon + \frac{v}{2}, \\ \beta_2 &= \epsilon - \frac{v}{2}, \\ \epsilon &= (E_i - E_f)/v, \\ N(v) &= \exp(\pi\nu/2) \Gamma(1 - i\nu), \\ v &= 1/v. \end{aligned} \quad (2)$$

The phase factor involved in the transition probability has been neglected because this does not contribute to the cross sections.  $\Phi_i$ ,  $\Phi_f$ ,  $E_i$ , and  $E_f$  are the wave functions and the corresponding electronic energies of the hydrogen atom in the initial and final states and  $\vec{\eta}$  is the transverse momentum transfer perpendicular to the incident velocity  $\vec{v}$ .

The total capture cross section  $Q_{if}$  is defined as

$$Q_{if}(a_0^2) = \int |T_{if}/2\pi v|^2 d\vec{\eta}. \quad (3)$$

### B. Evaluation of the integral $I$

The ground-state wave function of the target atom is

$$\Phi_i(\vec{x}) = \frac{1}{\sqrt{\pi}} (z_T)^{3/2} e^{-z_T x}, \quad (4)$$

the nuclear charge  $z_T$  of the target atom being unity. The  $I$  integral in Eq. (2) becomes

$$I = -\frac{1}{\sqrt{\pi}} (z_T)^{3/2} \frac{\partial}{\partial z_T} \int d\vec{x} \frac{e^{-z_T x + i\vec{p}\cdot\vec{x}}}{x} \times {}_1F_1(i\nu, 1; i\nu\vec{x} + i\vec{v}\cdot\vec{x}). \quad (5)$$

The above integral can be easily evaluated<sup>20</sup> as

$$I = -4\sqrt{\pi} (z_T)^{3/2} \frac{\partial}{\partial z_T} \frac{1}{(p^2 + z_T^2)} \times \left[ 1 - \frac{2(i\nu z_T - \vec{p}\cdot\vec{v})}{(p^2 + z_T^2)} \right]. \quad (6)$$

### C. Evaluation of the integral $I'$

The final bound-state wave function of the hydrogen atom specified by the set of quantum numbers  $n$ ,  $l$ , and  $m$  is given by

$$\Phi_{nlm}(\vec{s}) = N_{nlm} R_{nl}(s) Y_{lm}(\hat{s}), \quad (7)$$

where the normalization constant

$$N_{nlm} = -\frac{(2\gamma_n)^{l+1}}{(n+l)!} \left[ \frac{\gamma_n (n-l-1)!}{n(n+l)!} \right]^{1/2}, \quad (8)$$

with  $\gamma_n = 1/n$  and  $R_{nl}(s)$  and  $Y_{lm}(\hat{s})$  represent, respectively, the radial wave function and the spherical harmonics. We use the integral representation<sup>24</sup> of the Laguerre polynomial contained in  $R_{nl}(s)$  and obtain the  $I'$  integral in Eq. (2) as

$$I' = -N_{nlm} (n+l)! \frac{1}{2\pi i} \oint_c \frac{dt}{(1-t)^{2l+2} t^{n-l}} J, \quad (9)$$

with

$$J = \int d\vec{s} e^{-\mu s + i\vec{q}\cdot\vec{s}} s^{l-1} Y_{lm}^*(\hat{s}), \quad (10)$$

$$\mu = \gamma_n \left[ \frac{1+t}{1-t} \right]. \quad (11)$$

The angular integration in Eq. (10) can be performed easily and we arrive at

$$J = 4\pi i^l Y_{lm}^*(\hat{q}) \int_0^\infty j_l(qs) s^{l+1} e^{-\mu s} ds. \quad (12)$$

The radial integration in Eq. (12) is of standard form<sup>25</sup> and the  $J$  integral reduces to

$$J = 4\pi (l!) i^l Y_{lm}^*(\hat{q}) (2q)^l / (\mu^2 + q^2)^{l+1}. \quad (13)$$

Substituting the value of  $J$  from Eq. (12) into Eq. (9), we get

TABLE I. Capture cross sections  $n^3 \sigma_n$  (in units of  $10^{-16} \text{ cm}^2$ ) in the CISA method for  $\text{H}^+ \text{-H}$  collisions. The last column represents the asymptotic capture cross section  $n^3 \sigma_{n \rightarrow \infty, l}$  values,  $\sigma_n$  being the cross sections due to the quantum numbers  $n$  and  $l$ . The numbers in parenthesis are exponents of multiplicative factors of 10.

$E$ (keV)	$n$												
	$l$	0	1	2	3	0	1	2	3				
25		9.472 (0)	1.539 (1)	3.244 (0)	1.631 (-1)	9.700 (0)	1.585 (1)	3.836 (0)	3.200 (-1)	9.779 (0)	1.600 (1)	4.041 (0)	3.817 (-1)
50		1.574 (0)	2.107 (0)	3.818 (-1)	1.668 (-2)	1.630 (0)	2.227 (0)	4.961 (-1)	3.439 (-2)	1.649 (0)	2.269 (0)	5.009 (-1)	4.177 (-2)
100		1.456 (-1)	1.242 (-1)	1.544 (-2)	4.712 (-4)	1.500 (-1)	1.318 (-1)	1.921 (-2)	9.925 (-4)	1.516 (-1)	1.344 (-1)	2.059 (-2)	1.216 (-4)
250		2.719 (-3)	1.046 (-3)	6.360 (-5)	9.709 (-7)	2.767 (-3)	1.100 (-3)	7.895 (-5)	2.055 (-6)	2.785 (-3)	1.120 (-3)	8.458 (-5)	2.519 (-6)
500		8.403 (-5)	1.654 (-5)	5.371 (-7)	4.431 (-9)	8.489 (-5)	1.730 (-5)	6.640 (-7)	9.368 (-9)	8.520 (-5)	1.757 (-5)	7.106 (-7)	1.147 (-8)
750		9.741 (-6)	1.279 (-6)	2.823 (-8)	1.592 (-10)	9.813 (-6)	1.334 (-6)	3.486 (-8)	3.365 (-10)	9.836 (-6)	1.354 (-6)	3.727 (-8)	4.120 (-10)
1000		2.034 (-6)	1.993 (-7)	3.328 (-9)	1.426 (-11)	2.045 (-6)	2.076 (-7)	4.104 (-9)	3.011 (-11)	2.049 (-6)	2.106 (-7)	4.389 (-9)	3.687 (-11)
2500		1.213 (-8)	4.587 (-10)	3.081 (-12)	5.385 (-15)	1.216 (-8)	4.767 (-10)	3.793 (-12)	1.136 (-14)	1.216 (-8)	4.829 (-10)	4.051 (-12)	1.390 (-14)
5000		2.338 (-10)	4.220 (-12)	1.402 (-14)	1.228 (-17)	2.341 (-10)	4.380 (-12)	1.724 (-14)	2.588 (-17)	2.341 (-10)	4.438 (-12)	1.842 (-14)	3.168 (-17)
7500		2.291 (-11)	2.664 (-13)	5.834 (-16)	3.400 (-19)	2.292 (-11)	2.765 (-13)	7.173 (-16)	7.167 (-19)	2.293 (-11)	2.800 (-13)	7.660 (-16)	8.770 (-19)
10000		4.399 (-12)	3.732 (-14)	6.068 (-17)	2.645 (-20)	4.400 (-12)	3.873 (-14)	7.460 (-17)	5.553 (-20)	4.401 (-12)	3.922 (-14)	7.967 (-17)	6.820 (-20)

TABLE I. (Continued.)

$E$ (keV)	10			15			20			$\infty$						
	0	1	2	3	0	1	2	3	0	1	2	3				
25	9.812 (0)	1.608 (1)	4.134 (0)	4.114 (-1)	9.848 (0)	1.615 (+1)	4.226 (0)	4.414 (-1)	9.856 (0)	1.617 (1)	4.258 (0)	4.594 (-1)	9.874 (0)	1.620 (1)	4.300 (0)	4.658 (-1)
50	1.658 (0)	2.288 (0)	5.157 (-1)	4.539 (-2)	1.667 (0)	2.308 (0)	5.306 (-1)	4.911 (-2)	1.670 (0)	2.315 (0)	5.358 (-1)	5.043 (-2)	1.674 (0)	2.32 (0)	6.896 (-1)	5.217 (-2)
100	1.524 (-1)	1.357 (-1)	2.125 (-2)	1.324 (-3)	1.531 (-1)	1.370 (-1)	2.190 (-2)	1.437 (-3)	1.534 (-1)	1.374 (-1)	2.214 (-2)	1.478 (-3)	1.537 (-1)	1.380 (-1)	2.243 (-2)	1.531 (-3)
250	2.793 (-3)	1.129 (-3)	8.727 (-5)	2.748 (-6)	2.801 (-3)	1.138 (-3)	8.994 (-5)	2.986 (-6)	2.803 (-3)	1.142 (-3)	9.248 (-5)	3.071 (-6)	2.807 (-3)	1.145 (-3)	9.209 (-5)	3.183 (-5)
500	8.533 (-5)	1.770 (-5)	7.330 (-7)	1.252 (-8)	8.546 (-5)	1.782 (-5)	7.550 (-7)	1.360 (-8)	8.552 (-5)	1.786 (-5)	7.625 (-7)	1.398 (-8)	8.558 (-5)	1.792 (-5)	7.725 (-7)	1.449 (-8)
750	9.848 (-6)	1.363 (-6)	3.841 (-8)	4.495 (-10)	9.858 (-6)	1.372 (-6)	3.956 (-8)	4.880 (-10)	9.864 (-6)	1.374 (-6)	3.995 (-8)	5.019 (-10)	9.867 (-6)	1.379 (-6)	4.046 (-8)	5.200 (-10)
1000	2.051 (-6)	2.120 (-7)	4.522 (-9)	4.022 (-11)	2.053 (-6)	2.133 (-7)	4.654 (-9)	4.367 (-11)	2.054 (-6)	2.138 (-7)	4.702 (-9)	4.491 (-11)	2.054 (-6)	2.143 (-7)	4.763 (-9)	4.653 (-11)
2500	1.217 (-8)	4.858 (-10)	4.173 (-12)	1.516 (-14)	1.217 (-8)	4.887 (-10)	4.296 (-12)	1.646 (-14)	1.218 (-8)	4.898 (-10)	4.338 (-12)	1.693 (-14)	1.218 (-8)	4.910 (-10)	4.393 (-12)	1.753 (-14)
5000	2.342 (-10)	4.464 (-12)	1.897 (-14)	3.455 (-17)	2.342 (-10)	4.489 (-12)	1.952 (-14)	4.425 (-17)	2.342 (-10)	4.498 (-12)	1.971 (-14)	3.857 (-17)	2.342 (-10)	4.510 (-12)	1.996 (-14)	3.995 (-17)
7500	2.294 (-11)	2.817 (-13)	7.891 (-16)	9.566 (-19)	2.294 (-11)	2.832 (-13)	8.120 (-16)	1.038 (-18)	2.294 (-11)	2.838 (-13)	8.200 (-16)	1.068 (-18)	2.294 (-11)	2.846 (-13)	8.305 (-16)	1.106 (-18)
10000	4.402 (-12)	3.944 (-14)	8.206 (-17)	7.438 (-20)	4.401 (-12)	3.966 (-14)	8.444 (-17)	8.073 (-20)	4.402 (-12)	3.974 (-14)	8.528 (-17)	8.304 (-20)	4.402 (-12)	3.984 (-14)	8.635 (-17)	8.602 (-20)

$$I' = -N_{nlm} 4\pi(l!) i^l Y_{lm}^*(\hat{q}) (2q)^l [(n+l)!] \\ \times \frac{1}{2\pi i} \oint_c \frac{F(t) dt}{t^{n-l}}, \quad (14)$$

where

$$F(t) = A^{-l+1} (1-2Bt+t^2)^{-(l+1)}, \quad (15)$$

$$A = q^2 + \gamma_n^2, \quad (16)$$

$$B = (q^2 - \gamma_n^2)/A. \quad (17)$$

We express  $F(t)$  in terms of a Gegenbauer polynomial<sup>26</sup> and the contour integration in Eq. (14) can be performed easily. We obtain

$$I' = -N_{nlm} [(n+l)!] 4\pi(l!) i^l Y_{lm}^*(\hat{q}) (2q)^l \\ \times C_{n-l-1}^{l+1}(\lambda) A^{-(l+1)}. \quad (18)$$

Expressing the Gegenbauer polynomial in terms of hypergeometric series, we get

$$I' = S \cdot 2^{2l+3} \frac{\pi(l!) i^l}{(2l+1)!} Y_{lm}^*(\hat{q}) q^l A^{-(l+1)} \\ \times {}_2F_1 \left[ a, b, c, \frac{1-\lambda}{2} \right], \quad (19)$$

with

$$S = \gamma_n^{3/2} \left[ \prod_{r=0}^l (1 - \gamma_n^2 r^2) \right]^{1/2}, \quad (20)$$

$$a = n + l + 1, \quad (21)$$

$$b = -n + l + 1, \quad (22)$$

$$c = l + \frac{3}{2}. \quad (23)$$

### III. ASYMPTOTIC FORM OF THE SCATTERING AMPLITUDE

The behavior of the asymptotic cross sections for capture into any angular momentum states is of great importance. It has been found that  $S^{-1}I'$  is almost independent of the principal quantum number  $n$  in the intermediate- and high-energy region of the projectile and with the increase of  $n$ ,  $S^{-1}I'$  quickly approaches the limiting values as  $n \rightarrow \infty$ . With the increase of the principal quantum number  $n$  we get

$$\lim_{n \rightarrow \infty} \gamma_n = 0. \quad (24)$$

The limiting values of  $S^{-1}I'$  are obtained as

$$(S^{-1}I')_{n \rightarrow \infty} = 8\pi i^l Y_{lm}^*(\hat{q}) q^{-2} j_l(2/q).$$

Using Eqs. (1), (3), (6), and (25), the asymptotic capture cross sections can be found easily for any angular momentum state.

### IV. RESULTS AND DISCUSSION

The results of our numerical calculations of the integrated cross sections for electron capture by fast protons into arbitrary  $n$ ,  $l$ , and  $m$  state from the ground state of atomic hydrogen have been presented in Table I. To obtain the total cross section, the integration over the trans-

verse momentum transfer  $\eta$  has been performed numerically by the Gauss-Legendre quadrature method. The value of  $\eta$  has been increased stepwise until the desired accuracy of 0.5% in the total capture cross sections is obtained. As a numerical check on our general computer program all the earlier results for the low-lying states reported by Belkić<sup>20</sup> have been reproduced.

From the table it is interesting to note that the  $n^3$ -times cross section for different values of  $l$  tends to a constant value in a consistent manner with the increase of  $n$  at each incident energy depending only on the energy of the projectile. The values of the  $n^3$ -times cross section for  $n=20$  are in close agreement with the asymptotic cross-section values at all energies. Thus the  $n^{-3}$  law is obeyed by the CISA cross section throughout the energy range of the projectile considered and this behavior is in correspondence with the previous investigation.<sup>8,9</sup> However, this law has been found to be satisfied more significantly by the FBA, SBA, and EA calculations as compared to the present CISA calculation. The present CISA cross sections are found to decrease rapidly with the increase of the energy. In general, the cross sections decrease rapidly with the increase of  $l$ . However, the cross sections for the  $np$  state are found to be larger than those of the  $ns$  state in the intermediate-energy region, whereas the cross sections for  $l=0$  states are found to be larger in the high-energy region. Although we have not shown in the present table the  $m$ -dependent cross sections, it has been found that the

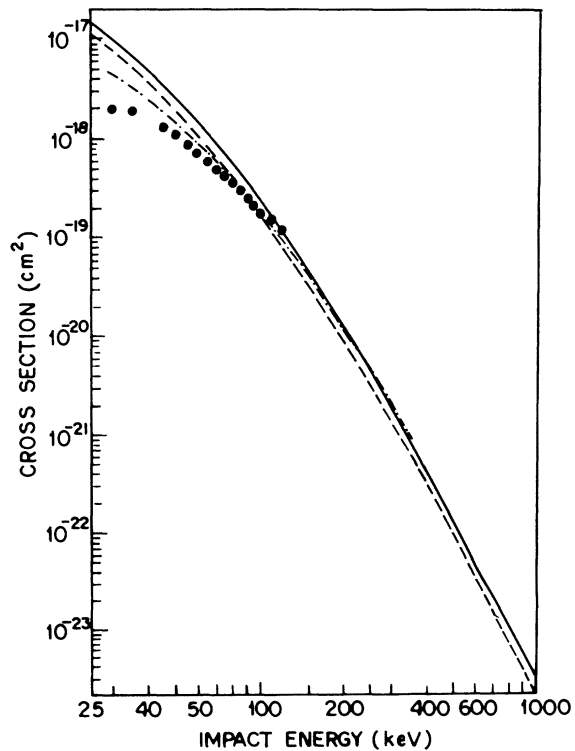


FIG. 1. Cross sections for electron capture by protons in the 4s state from the ground state of atomic hydrogen. Theory: solid curve, present work; dashed curve, Belkić and Gayet (Ref. 18); dashed-dotted curve, Chan and Eichler (Ref. 12). Experiment:  $\circ$ , Hughes *et al.* (Ref. 27).

cross sections for the  $m=0$  state for a given  $n$  and  $l$  are maximum.

The asymptotic capture cross-section data are extremely useful for giving a reliable estimate for capture into excited states with moderate and high values of  $n$ , since  $S^{-1}I'$  has been found to be more or less constant at high energies. To obtain the  $n^3$  cross section for capture into the " $n$ " state, the asymptotic  $n^3$  capture cross section for a particular angular momentum state should be multiplied by the factor

$$\sum_{r=0}^l (1 - r^2/n^2).$$

Obviously, a better result is expected for large values of  $n$  and with the increase of the incident energy of the projectile. However, at intermediate energies and moderate values of  $n$ , this rule may be applied with a sufficient limit of accuracy. For comparison with the actual calculations we have calculated the values of cross sections for a few excited states by applying the above rule (not shown in the table). The close agreement between these results indicate the applicability of the scaling rule in prediction of the various cross sections for capture into different angular momentum states.

In Fig. 1 we compare our present results for capture in the  $4s$  excited state with the CDWA (Ref. 18) and the EA (Ref. 12) calculations as well as with the experimental data

of Hughes *et al.*<sup>27</sup> The present calculation is found to be in quite good agreement with the measurements. The CISA results slightly overestimate the cross sections calculated by the CDWA approach. This overestimation is in correspondence with the previous investigation<sup>20</sup> for capture in the  $2s$  and  $3s$  excited states of atomic hydrogen. However, the EA (Ref. 12) results are closer to the experimental values as compared to the CDWA and CISA calculations.

## V. CONCLUDING REMARKS

A new straightforward method for the evaluation of the CISA scattering amplitude has been developed without imposing any restrictions on the values of the quantum numbers  $n$ ,  $l$ , and  $m$  of the excited states of atomic hydrogen. The scattering amplitude is reduced to a closed analytical form which can easily be evaluated numerically and requires little computation time. The asymptotic form of the scattering amplitude as  $n \rightarrow \infty$  may be obtained without encountering any further difficulties. The data of the asymptotic capture cross sections are useful to give an estimate of the cross sections into various excited levels with the help of a simple rule. For capture into highly excited states, the  $n^{-3}$  law for the CISA cross section for the electron capture into any angular momentum states is found to be satisfied at all incident energies.

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